“Design, Synthesis and Investigation of Potential Bioactive Pharmacophores Derived From Different Simple and Fused Heterocycles.”

A synopsis submitted to

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Title of the Proposed Research Work:

"Design, Synthesis and Investigation of Potential Bioactive Pharmacophores Derived From Different Simple and Fused Heterocycles."

1. Introduction:

Heterocyclic compounds constitute the largest and most varied family of organic compounds. Many broader aspects of heterocyclic chemistry are recognized as disciplines of general significance that impose on almost all aspects of modern organic chemistry, medicinal chemistry and biochemistry. Heterocyclic compounds offer a high degree of structural diversity and have proven to be broadly and economically useful as therapeutic agents.[1]

Heterocyclic compounds containing –SH, NH, N-C-S, NH-R and N-C=S, groups in a ring have an important role inorganic synthesis and medicinal chemistry due to their considerable bioactivity. It makes possible research, upgrading the synthesis, modification and changes in structure of heterocyclic compounds. The compounds are also accompanied by changing the biological activity. Many naturally occurring and synthetic compounds containing Nitrogen, Sulfur and Oxygen elements possess interesting pharmacological properties. They are continuing to be in the focus of life science-oriented research.

Synthetic medicinal chemistry is principally concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships. Medicinal chemistry involves the identification, synthesis and development of new chemical entities suitable for therapeutic use. Generally, synthesis is based on the designing and synthesis of different novel compounds through structural modification of some already existing chemical entities. Modifications involved in medicinal chemistry are usually made with objective of improving potency, safety and economic profile of already existing compounds. Today more than 60% drugs used in practice are synthetic derivatives and

day-by-day the scope of medicinal chemistry is broadening. Medicinal chemistry according to Burger, ***"tries to be based on the ever-increasing hope that biochemical rationales for drug discovery may be found"*** Synthetic drug however containing various mechanisms in human bodies to prevent their excessive actions have a single mode of action and may cause a severe adverse reaction when given in large doses or for a long period of time or sometimes differ with individuals or a reason of faulty diagnosis.

Organic synthesis is one of the special branches in chemical synthesis and is concerned with the construction of organic compounds by reactions. It is believed to be one of the most vital in organic chemistry because the organic molecules used to contain higher level of complexity compared to pure inorganic compounds.

Hence, we aimed to study and development of new heterocyclic derivatives by using structural modification strategy, molecular hybridization (MH) or hybrid based heterocyclic.

Design of new drugs with better physicochemical properties, adequate absorption, distribution, metabolism and excretion along with effective pharmacologic potency and lack of toxicity for the treatment of infectious diseases has suffered a continuous decrease.

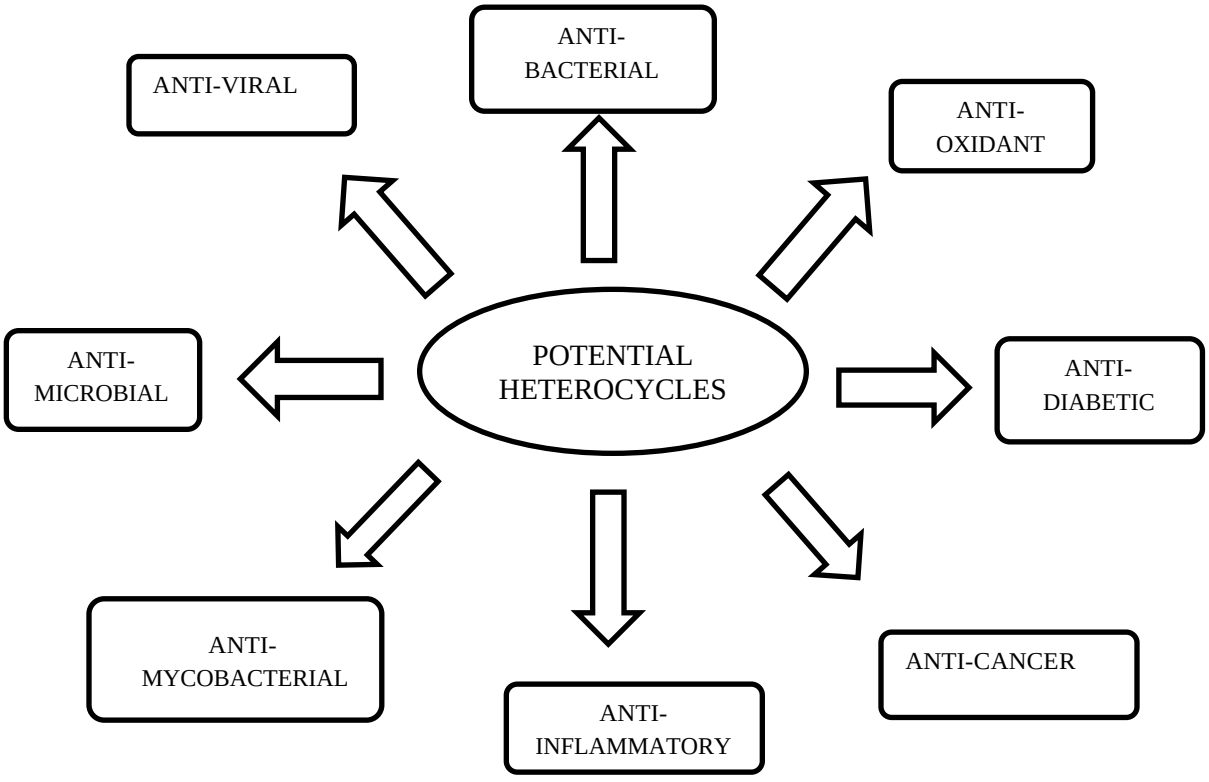


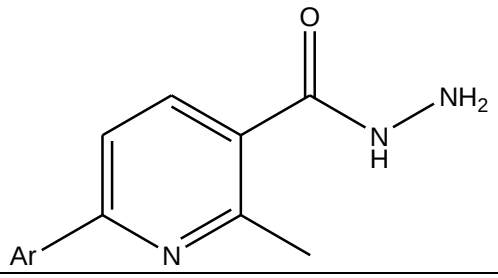
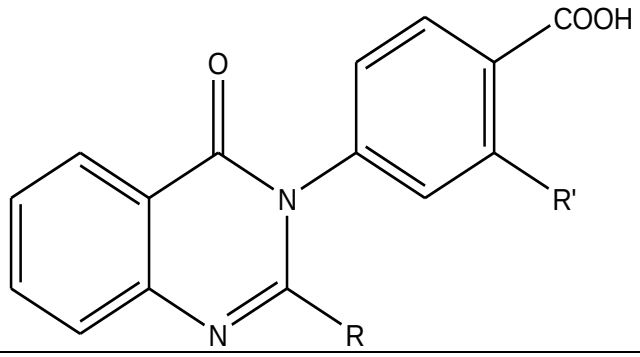
Figure 1 Biological Activities of Heterocyclic compounds

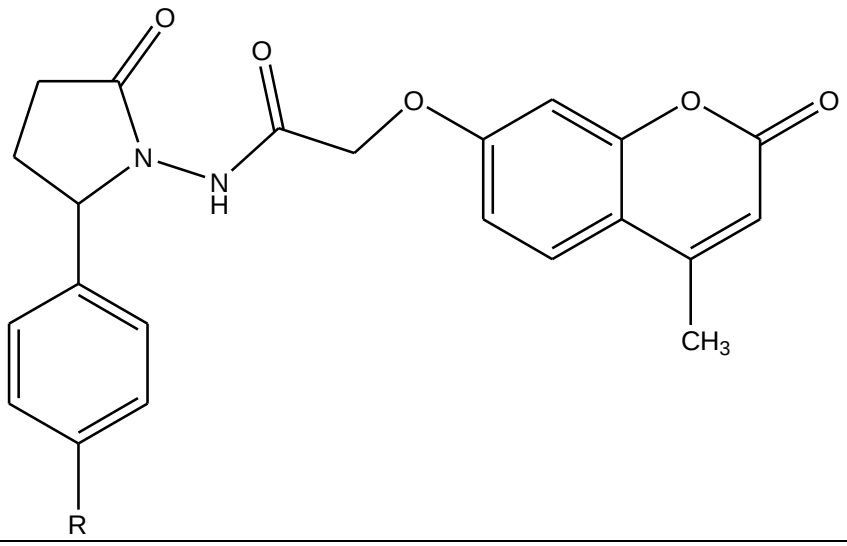
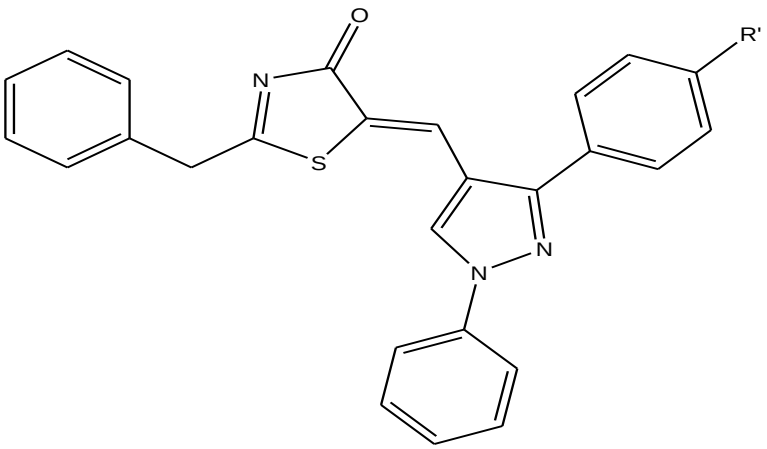
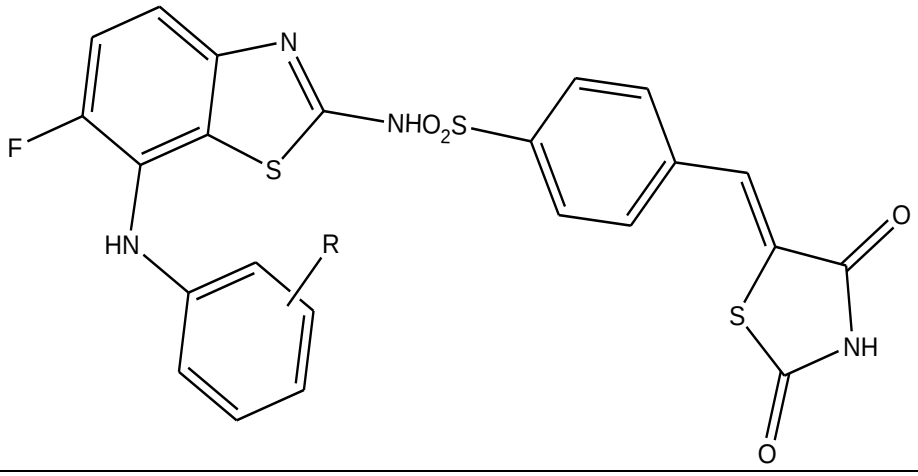
The synthesis of derivatives has been an important part and is aimed at modifying the action of drugs, particularly to reduce the side effects and to potentiate the drug action. Nitrogen, oxygen and Sulphur are the most common heteroatoms, but heterocyclic rings containing other hetero atoms are also widely known. A enormous number of heterocyclic compounds are known and this number is increasing rapidly.

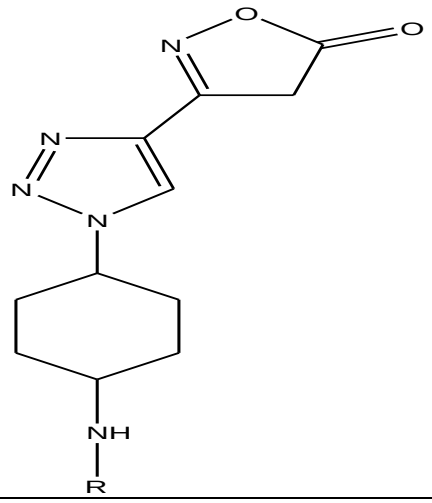
2. Review of Literature and Development in the subject:

In recent years heterocyclic compounds are being actively studied by many research groups. Heterocycles and their analogues have important and wide application in organic chemistry, medicinal chemistry and pharmaceutical industries.

Various heterocycles showing their broad-spectrum applications such as:

Sr no	Heterocyclic moiety	Biological Activity
1.		Antitubercular[2]
2.		Antiviral[3]

3.		Antioxidant and Anticancer[4]
4.		Antimicrobial and Anticancer[5]
5.		Antidiabetic[6]

6.		Antifungal[7]

3. Objective of research/ Proposed Hypothesis:

1) To design potential derivatives.
2) To synthesize some newer derivatives.
3) To characterize the synthesized compounds by different analytical techniques such as IR, NMR and Mass spectral data.
4) To screen the synthesized compounds for their biological activities.
5) To publish the research works in peer reviewed journals.

4. Methodology to be adopted:

A) Designing and Synthesis of the compounds:

Chemicals and other reagents required for the synthesis will be procured from standard company sources. Compounds will be synthesized by standard procedures given in the literature and proposed method. The reactions will be monitored by TLC and purification of the compounds will be carried out by recrystallization method using suitable solvent.

B) Characterization of the compounds:

The synthesized compounds will be characterized by preliminary laboratory techniques such as

melting point, boiling point etc. and by FTIR, Mass Spectroscopy and NMR spectral data.

C) Biological Evaluation:

The synthesized compounds shall be evaluated for their different biological activity.

5. Importance of study/society applications:

5.1 International Status :

From many decades, world facing the outbreak of pandemic diseases like COVID-19, AIDS and Flue. Such a pandemic conditions increase the rate of mortality result in the deaths of more than 38 million of peoples. During the period researchers dispense the new drugs out of which 90% of drugs used in pandemic conditions are heterocyclic compounds.

5.2 National Status :

At National level the significance of heterocyclic compounds has been growing interest in the scientific community be speak to have opportunity for design, synthesis and investigation of Potential Bioactive Pharmacophores Derived from Different Simple and Fused Heterocycles."

5.3. Significance of the study:

The potential significance of active heterocycles has been growing interest inthe scientific community and motivated to opportunity form research work.

With the given background and motivation, I would like to focus on hybrid-based heterocycles and their derivatives have significant and potential application in various fields

6. Proposed work plan/Formulation of structured study:

1) To carry out the comprehensive literature survey.
2) To establish the method of synthesis and designing for the proposed compounds.
3) To synthesize proposed compounds by appropriate method.

4) To confirm the structure of the synthesized compound by spectroscopy.
5) To evaluate the proposed compounds for a biological activity by the known standard method.

7.References:

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